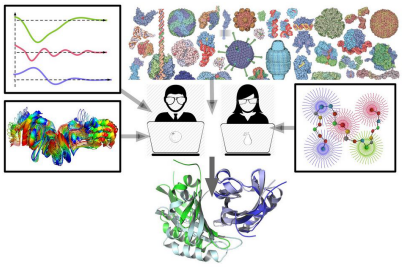

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DECOMPOSITION OF EVOLVING SAXS DATASETS USING CHEMOMETRICS

Many biologically important systems are inherently polydisperse e.g. transient protein-protein complexes, oligomerizing proteins or proteins with different co-existing conformations. Such systems are always in an equilibrium of different species and are therefore heterogenous. Importantly, such systems can't be meaningfully studied in a holistic sense by physically separating the components of the system as they exist in context of each other. Small Angle X-ray Scattering (SAXS) is an excellent tool to study such systems as SAXS data is additive and in principle, can be decomposed into the scattering profiles of the components. We have developed a chemometrics based, model free method to decompose evolving SAXS datasets into the SAXS profiles of the individual components and recover the relative populations at the same time1. Our method can use multiple SAXS datasets and multiple representation of the SAXS profiles to improve the resolution of the curves and reduce the ambiguity of the solutions.
Our tests on simulated SAXS titrations datasets of transient protein-protein complexes demonstrate that we are able to recover the SAXS profile, and therefore the size and shape parameters, of the complex. At the same time, we are also able to extract the fractions of the complex and the dissociated components through the titration series, giving insight into the thermodynamics of the system.
Our approach would be useful to study a variety of evolving SAXS data sets (Oligomerization, Titrations of transient complexes, Time-resolved SAXS, Fibrillation, etc.) and extends the reach of SAXS into the realm of complex, heterogeneous, evolving biological systems.

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